

Evaluation of overlaps between arbitrary Fermionic quasiparticle vacua

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We derive an expression that allows for the unambiguous evaluation of the overlap between two arbitrary quasiparticle vacua, including its sign. Our expression is based on the Pfaffian of a skew-symmetric matrix, extending the formula recently proposed by [L. M. Robledo, Phys. Rev. C **79**, 021302(R) (2009)] to the most general case, including the one of the overlap between two different blocked n -quasiparticle states for either even or odd systems. The powerfulness of the method is illustrated for a few typical matrix elements that appear in realistic angular-momentum-restored Generator-Coordinate Method calculations when breaking time-reversal invariance and using the full model space of occupied single-particle states.

I. INTRODUCTION

The evaluation of kernels in projection and more general applications of the Generator Coordinate Method (GCM) based on quasiparticle vacua requires the calculation of the overlap between two different quasiparticle vacua. Its evaluation presents a long-standing technical challenge: the standard expression for this overlap, the so-called "Onishi formula" [1] provides the square of the (complex) overlap only. As a consequence, the overall sign of the overlap is not determined, or, equivalently, its phase is determined up to integer multiples of π only.

One possible solution to the problem was proposed by Neergård and Wüst [2], but the practical application of their technique becomes cumbersome in realistic applications and has been rarely used in practice. Notable exceptions are Refs. [3, 4]. Many groups have resided to determine the phase through a kind of Taylor expansion that allows "to follow the overlap" when the kernel can be connected in small steps to a known reference overlap (see, for example, Refs. [5, 6]). In practice this can become very cumbersome or even impossible when the phase is rapidly changing or when there is no symmetry that establishes a reference phase.

It was pointed out by Robledo in Ref. [7] that techniques for the manipulation of matrix elements between Fermionic coherent states that are well-known in field theory allow to express the overlap between two quasiparticle vacua, including its sign, as the so-called Pfaffian of a skew-symmetric matrix.¹ In a more recent paper, Robledo [9] has also worked out the practical implementation of this idea for the unambiguous evaluation of the overlap between fully-paired quasiparticle vacua, including the limit where some of the "pairs" consist of fully occupied single-particle states. Even more recently, Bertsch and Robledo [10] also investigated the case of systems with an odd number of constituents, providing the un-

ambiguous evaluation of the overlap for the special case of two quasiparticle vacua linked by a symmetry transformation.

In the present paper, we present the extension of this scheme to the calculation of the overlap between two possibly different arbitrary quasiparticle vacua, generalizing the treatment of completely filled single-particle states to the most general case. This extension thus allows to handle quasiparticle vacua obtained from blocked 1-, 2-, \dots n arbitrary quasiparticle states. To this aim, we present an alternative derivation of the overlap that makes use of an extension of the standard Thouless parameterization of quasiparticle vacua [11] that is advantageous in the presence of completely filled single-particle states and allows to avoid many of the matrix manipulations elaborated in Ref. [9]. Also, our final expression Eq. (63) allows for the calculation of the overlap of two quasiparticle vacua that are expressed in different single-particle bases that do not span the same sub-space of the Hilbert space of single-particle states, a situation frequently encountered in symmetry-restored GCM codes that use a coordinate space representation of the quasiparticle vacua in terms of their canonical single-particle bases [12–16].

The article is organized as follows: Section II introduces a generalization of the Thouless parameterization of quasiparticle vacua for blocked states that will turn out to be useful for the purpose of our paper. Section III reviews key properties of Fermionic coherent states and Grassmann calculus that will be needed later on and thereby introduces our notation. Section IV describes the calculation of the overlap, and Section V presents some illustrative examples of overlaps from realistic calculations. Finally, Section VI summarizes our findings. An appendix gives the representation of determinants and Pfaffians of skew-symmetric matrices in terms of integrals over Grassmann variables.

II. PARAMETERIZATION OF QUASIPARTICLE VACUA

Let $\{\hat{a}^\dagger, \hat{a}\}$ and $\{\hat{b}^\dagger, \hat{b}\}$ be two not necessarily equivalent single-particle bases of dimension n (n even), with

¹ The possibility to use Pfaffians for this purpose was already conjectured much earlier by Balian and Brézin in Ref. [8], but never worked out.

which are defined two (not normalized) quasiparticle vacua $|\phi_a\rangle$ and $|\phi_b\rangle$ through the parameterizations²

$$|\phi_c\rangle = e^{\frac{1}{2} \sum_{kl} M_{kl}^{(c)} \hat{c}_k^\dagger \hat{c}_l^\dagger} \prod_{i \in \{I^c\}}^{\triangleright} \hat{c}_i^\dagger |-\rangle, \quad (1)$$

where c is either a or b , $|-\rangle$ is the bare vacuum of single-particle operators, and where the $M^{(c)}$ are skew-symmetric matrices. Their elements with indices belonging to the ensemble of fully occupied states $\{I^c\}$ of cardinality³ $\#I^c = r_c$ are (can be) put to zero. This constitutes a natural way to regularize the matrix $M^{(c)}$ in the presence of fully-occupied states.

The triangle pointing to the right on top of the product sign means that it is a "direct" product,

$$\prod_{i \in \{I^c\}}^{\triangleright} \hat{c}_i^\dagger = \hat{c}_\mu^\dagger \cdots \hat{c}_\nu^\dagger \hat{c}_\delta^\dagger, \quad \text{with } \mu > \cdots > \nu > \delta, \quad (2)$$

as opposed to a "reverse" product obtained, for example, by taking the adjoint of Eq. (2), i.e.

$$\prod_{i \in \{I^c\}}^{\triangleleft} \hat{c}_i = \hat{c}_\delta \hat{c}_\nu \cdots \hat{c}_\mu, \quad \text{with } \mu > \cdots > \nu > \delta. \quad (3)$$

The parameterization Eq. (1) of quasiparticle vacua is not very different from the one by Thouless [11]. However, it has two advantages important for our purpose. First, this parameterization is well-defined when dealing with fully occupied states. And second, it allows to parameterize a quasiparticle vacuum for systems with odd particle number in terms of single-particle states, something that cannot be achieved with the standard Thouless formula. However, this parameterization can be set-up only in a specific single-particle basis that separates the fully-occupied single-particle states from the others. Such a single-particle basis is, for example, the canonical single-particle basis of a quasiparticle vacuum. The use of these bases does not impose a serious restriction, since they provide the most compact representation of a quasiparticle vacuum, such that their use is often desirable in numerical applications.

Finally, the convention for the ordering of single-particle levels in Eq. (1) (matrix elements of $M^{(c)}$ and product ordering) is to be kept unchanged for *each* calculation involving a given state $|\phi_c\rangle$. In fact, Eq. (1) is just an alternative convention that circumvents the convention of Ref. [7] to connect the phase of $\langle\phi_a|\phi_b\rangle$ to $\langle\phi_a|-\rangle$ and $\langle-|\phi_b\rangle$, which cannot be achieved when either $\langle\phi_a|-\rangle$ or $\langle-|\phi_b\rangle$ (or both) is (are) zero.

III. A REMINDER ON FERMIONIC COHERENT STATES AND GRASSMANN CALCULUS

In order to evaluate the overlap $\langle\phi_a|\phi_b\rangle$ between the two states, we introduce, following closely Ref. [7], two sets of Fermionic coherent states

$$|z_c\rangle = e^{\hat{c}^\dagger \cdot z_c} |-\rangle \quad (4)$$

$$\langle z_c| = \langle -| e^{\bar{z}_c \cdot \hat{c}} \quad (5)$$

for $c = a, b$, parameterized in terms of anticommuting z_{c_k} and \bar{z}_{c_k} elements of a Grassmann algebra \mathcal{G} , where the notations $\hat{c}^\dagger \cdot z_c$ and $\bar{z}_c \cdot \hat{c}$ used in Eq. (4) and Eq. (5) stand for

$$\hat{c}^\dagger \cdot z_c = \sum_{i=1}^n \hat{c}_i^\dagger z_{c_i}, \quad (6)$$

$$\bar{z}_c \cdot \hat{c} = \sum_{i=1}^n \bar{z}_{c_i} \hat{c}_i. \quad (7)$$

In particular, we notice that the coherent states $|z_c\rangle$ are not normalized. Instead, one has $\langle -|z_c\rangle = \langle z_c|-\rangle = 1$.

In what follows, we recall some useful properties of Grassmann algebra, its associated calculus, and of Fermionic coherent states that will be needed for the formal derivations outlined below. Concerning Grassmann algebra and calculus [17–19], we recall that

- The adjoint operator performs a one-to-one mapping within \mathcal{G}

$$(z_{c_k})^\dagger = \bar{z}_{c_k}, \quad (8)$$

$$(\bar{z}_{c_k})^\dagger = z_{c_k}, \quad (9)$$

$$(z_{c_k} z_{c_l})^\dagger = \bar{z}_{c_l} \bar{z}_{c_k}. \quad (10)$$

- Grassmann variables anticommute

$$z_{c_k} z_{c_l} = -z_{c_l} z_{c_k}, \quad (11)$$

$$\bar{z}_{c_k} \bar{z}_{c_l} = -\bar{z}_{c_l} \bar{z}_{c_k}, \quad (12)$$

$$z_{c_k} \bar{z}_{c_l} = -\bar{z}_{c_l} z_{c_k}, \quad (13)$$

$$z_{c_k} z_{c_k} = \bar{z}_{c_k} \bar{z}_{c_k} = 0. \quad (14)$$

In the following, a product of p Grassmann variables (\mathcal{G} -variables) will be called a monomial of degree p . When p is even (odd), such a product will be called an even (odd) monomial. We notice that an even monomial of \mathcal{G} -variables commutes with even and odd monomials of \mathcal{G} -variables. We also remark that exponentials of pairs of \mathcal{G} -variables also commute with even and odd monomials of \mathcal{G} -variables, such an exponential being a sum of even monomials of \mathcal{G} -variables.

- \mathcal{G} -variables commute with complex numbers and anticommute with Fermionic operators.

² For time being, n will be the minimal number of single-particle states that allows to represent both $|\phi_a\rangle$ and $|\phi_b\rangle$ in their respective single-particle basis.

³ The cardinality is the number of elements of an ensemble.

- The fundamental Grassmann calculus rules are

$$\int dz_{c_k} z_{c_k} = \frac{\partial}{\partial z_{c_k}} z_{c_k} = 1, \quad (15)$$

$$\int dz_{c_k} = 0. \quad (16)$$

- As a consequence of Eq. (14), the \mathcal{G} -variables z_{c_k} play the role of their own δ -functions, e.g., for an analytic function f of \mathcal{G} -variables (c.f. [19], p. 91), we have

$$\int dz_{c_k} z_{c_k} f(z_{c_k}) = f(0). \quad (17)$$

- The *adjoint* variables \bar{z}_{c_k} and z_{c_k} are independent integration variables (c.f. [17], p. 28).

Concerning Fermionic coherent states, the properties to be used in what follows are:

- They are eigenstates of second quantized operators

$$\hat{c}_k |z_c\rangle = z_{c_k} |z_c\rangle, \quad \langle z_c | \hat{c}_k^\dagger = \langle z_c | \bar{z}_{c_k}, \quad (18)$$

with the eigenvalues being Grassmann variables.

- They resolve the identity through the closure relation

$$\mathbb{1}_c = \int d_{\triangleright}^n \bar{z}_c d_{\triangleleft}^n z_c |z_c\rangle e^{-\bar{z}_c \cdot z_c} \langle z_c|, \quad (19)$$

where $\mathbb{1}_c$ means that the resolution of the identity is built for Fock spaces generated by $\{\hat{c}^\dagger, \hat{c}\}$. We use the short-hand notation $\bar{z}_c \cdot z_c \equiv \bar{z}_c^t z_c = \sum_{i=1}^n \bar{z}_{c_i} z_{c_i}$. Finally, d_{\triangleright}^n and d_{\triangleleft}^n represent products of differential elements that are ordered such that

$$d_{\triangleright}^n \mathbf{x} = dx_n \cdots dx_2 dx_1, \quad (20)$$

$$d_{\triangleleft}^n \mathbf{x} = dx_1 dx_2 \cdots dx_n. \quad (21)$$

As compared to [7] and many textbooks, we change the ordering of the products of differential elements in the integral in order to anticommute them in a more transparent way, i.e. we use

$$d_{\triangleright}^n \bar{z}_c d_{\triangleleft}^n z_c, \quad (22)$$

which is equivalent to the more commonly used ordering⁴

$$\prod_i d\bar{z}_{c_i} dz_{c_i}. \quad (23)$$

IV. EVALUATION OF THE OVERLAPS

A. Preliminary considerations

To evaluate the expression for the overlap, we start by inserting two closure relations, the left (right) one being based on the single-particle basis of the left (right) state, e.g. $\langle \phi_a | \phi_b \rangle = \langle \phi_a | \mathbb{1}_a \mathbb{1}_b | \phi_b \rangle$

$$\begin{aligned} \langle \phi_a | \phi_b \rangle &= \int d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b d_{\triangleleft}^n z_b \\ &\times \langle \phi_a | z_a \rangle e^{-\bar{z}_a \cdot z_a} \langle z_a | z_b \rangle e^{-\bar{z}_b \cdot z_b} \langle z_b | \phi_b \rangle, \end{aligned} \quad (24)$$

where we implicitly use that $d_{\triangleright}^n \bar{z}_c d_{\triangleleft}^n z_c$ ($c = a, b$) are even $(2n)$ monomials of Grassmann differential elements, and thus commuting with Fermionic operators, in order to move all differential elements to the very left.

When the single-particle bases of a and b do not span the same subspace of the Hilbert space of single-particle states, e.g. when they are not linked through a unitary transformation, the resolution of the identity $\mathbb{1}_a$ ($\mathbb{1}_b$) works for the left (right) state alone, and the two closure relations are *not* equivalent. However, there is no loss of generality for the following, their non-equivalence being carried by the overlap kernel $\langle z_a | z_b \rangle$.

Given that by definition $\langle - | z_c \rangle = \langle z_c | - \rangle = 1$, we first evaluate the three overlaps

$$\langle \phi_a | z_a \rangle = \prod_{i \in \{I^a\}} z_{a_i} e^{-\frac{1}{2} \sum_{kl} M_{kl}^{(a)*} z_{a_k} z_{a_l}}, \quad (25)$$

$$\langle z_b | \phi_b \rangle = e^{+\frac{1}{2} \sum_{kl} M_{kl}^{(b)} \bar{z}_{b_k} \bar{z}_{b_l}} \prod_{j \in \{I^b\}} \bar{z}_{b_j}, \quad (26)$$

$$\langle z_a | z_b \rangle = e^{\sum_{kl} \bar{z}_{a_k} R_{kl} z_{b_l}}. \quad (27)$$

The two first expressions use the properties Eq. (18) of coherent states. The last one uses the Baker-Campbell-Hausdorff formula,⁵ such that

$$\begin{aligned} \langle z_a | z_b \rangle &= \langle - | e^{\bar{z}_a \cdot \hat{\mathbf{a}}} e^{\hat{\mathbf{b}}^\dagger \cdot z_b} | - \rangle \\ &= \langle - | e^{\hat{\mathbf{b}}^\dagger \cdot z_b} e^{\bar{z}_a \cdot \hat{\mathbf{a}}} e^{[\bar{z}_a \cdot \hat{\mathbf{a}}, \hat{\mathbf{b}}^\dagger \cdot z_b]} | - \rangle. \end{aligned} \quad (28)$$

Indeed, the latter is applicable because the commutator

$$[\bar{z}_a \cdot \hat{\mathbf{a}}, \hat{\mathbf{b}}^\dagger \cdot z_b] = \sum_{ij} \bar{z}_{a_i} \{ \hat{a}_i, \hat{b}_j^\dagger \} z_{b_j} \quad (29)$$

$$= \sum_{ij} \bar{z}_{a_i} R_{ij} z_{b_j} = \bar{z}_a^t R z_b, \quad (30)$$

commutes with $\bar{z}_a \cdot \hat{\mathbf{a}}$ and $\hat{\mathbf{b}}^\dagger \cdot z_b$, where $R_{ij} \equiv \{ \hat{a}_i, \hat{b}_j^\dagger \}$ denotes the matrix of overlaps of the single-particle states

⁴ In the commonly used ordering, there is no need to define a particular product ordering as $d\bar{z}_{c_i} dz_{c_i}$ are even monomials of \mathcal{G} -variables, and the overall order convention is carried only by $d\bar{z}_{c_i} dz_{c_i}$.

⁵ The Baker-Campbell-Hausdorff formula states that, if $[X, [X, Y]] = [Y, [Y, X]] = 0$, then $e^X e^Y = e^Y e^X e^{[X, Y]}$.

corresponding to \hat{a}_i and \hat{b}_j^\dagger . We finally obtain Eq. (27) by considering that $|-\rangle$ is a common vacuum for the operators \hat{a} and \hat{b} .

B. Integration of the reproducing kernel

As the next step, we integrate the expression for the reproducing kernel

$$e^{-\bar{z}_a \cdot z_a} \langle z_a | z_b \rangle e^{-\bar{z}_b \cdot z_b} = e^{-\bar{z}_a \cdot z_a + \bar{z}_a^t R z_b - \bar{z}_b \cdot z_b}, \quad (31)$$

where we use that exponentials of pairs of \mathcal{G} -variables commute, thereby allowing to merge the three exponential factors.

Noticing that, in Eq. (24), \bar{z}_a and z_b only appear in the reproducing kernel Eq. (31), we want to integrate these

variables separately. In order to do so, we first remark that the expression Eq. (31) can be moved to the very right of Eq. (24) because it commutes with \mathcal{G} -variables. We can as well move the product of differential elements $d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b$ in front of it by virtue of

$$\begin{aligned} \overbrace{d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b d_{\triangleleft}^n z_b} &= (-1)^{2n^2} d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b \\ &= d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b \underbrace{d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b}_{\text{even product}}. \end{aligned} \quad (32)$$

With $d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b$ being an even product of Grassmann differential elements, it commutes with $\langle \phi_a | z_a \rangle$ and $\langle z_b | \phi_b \rangle$, quantities containing neither the variables \bar{z}_a nor z_b , c.f. Eqns. (25) and (26). Rewriting Eq. (24) in a more suitable way now gives

$$\langle \phi_a | \phi_b \rangle = \int d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b \left(\langle \phi_a | z_a \rangle \langle z_b | \phi_b \rangle \underbrace{\left(\int d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b e^{-\bar{z}_a \cdot z_a + \bar{z}_a^t R z_b - \bar{z}_b \cdot z_b} \right)}_{\text{reproducing kernel integral}} \right). \quad (33)$$

We now evaluate the reproducing kernel integral. Provided that R is non-singular,^{6,7} we make the change of variables (c.f. Ref. [19] p. 14)

$$\begin{aligned} \bar{\eta}^t &= \bar{z}_a^t - \bar{z}_b^t R^{-1} \\ \eta &= z_b - R^{-1} z_a \end{aligned} \quad (34)$$

such that

$$\bar{\eta}^t R \eta = -\bar{z}_a \cdot z_a + \bar{z}_a^t R z_b - \bar{z}_b \cdot z_b + \bar{z}_b^t R^{-1} z_a. \quad (35)$$

The reproducing kernel can now be written

$$e^{-\bar{z}_a \cdot z_a + \bar{z}_a^t R z_b - \bar{z}_b \cdot z_b} = e^{-\bar{z}_b^t R^{-1} z_a} e^{\bar{\eta}^t R \eta}. \quad (36)$$

The Jacobian of the transformation being one, i.e. $d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b \equiv d_{\triangleright}^n \bar{\eta} d_{\triangleleft}^n \eta$, the integration gives

$$\begin{aligned} &\int d_{\triangleright}^n \bar{z}_a d_{\triangleleft}^n z_b e^{-\bar{z}_a \cdot z_a + \bar{z}_a^t R z_b - \bar{z}_b \cdot z_b} \\ &= e^{-\bar{z}_b^t R^{-1} z_a} \int d_{\triangleright}^n \bar{\eta} d_{\triangleleft}^n \eta e^{\bar{\eta}^t R \eta} \\ &= (-1)^n \det(R) e^{-\bar{z}_b^t R^{-1} z_a} \end{aligned} \quad (37)$$

where we have used the determinant formula outlined in Eq. (A2) of Appendix A.

⁶ The case of singular R is not equivalent of having zero overlap. As an example, consider the case of a partially or completely empty single-particle state of the left vacuum which is orthogonal to all single-particle states of the right vacuum. In this case, R is singular, whereas the overlap is not necessarily zero.

⁷ In case of singular R , one has to complete the single-particle bases of $|\phi_a\rangle$ and $|\phi_b\rangle$ in order to get an invertible matrix, for example using a Gram-Schmidt orthonormalization procedure. Still, having a non-singular matrix R is not equivalent to having equivalent bases a and b .

C. Re-expression of the overlap

Using Eqns. (25), (26) and (37), we are now able to rewrite Eq. (33) as

$$\langle \phi_a | \phi_b \rangle = (-1)^n \det(R) \int d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b \left(\langle \phi_a | z_a \rangle \langle z_b | \phi_b \rangle e^{-\bar{z}_b^t R^{-1} z_a} \right) \quad (38)$$

$$= (-1)^n \det(R) \int d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b \left(\prod_{i \in \{I^a\}}^{\triangleleft} z_{a_i} \prod_{j \in \{I^b\}}^{\triangleright} \bar{z}_{b_j} e^{\left(-\frac{1}{2} \sum_{kl} M_{kl}^{(a)*} z_{a_k} z_{a_l} + \frac{1}{2} \sum_{kl} M_{kl}^{(b)} \bar{z}_{b_k} \bar{z}_{b_l} - \bar{z}_b^t R^{-1} z_a\right)} \right) \quad (39)$$

where we used that exponentials of pairs of \mathcal{G} -variables commute with \mathcal{G} -variables. Closely following the notation of Ref. [7], we introduce the matrix \mathbb{M} and the vector ζ

$$\mathbb{M} \equiv \begin{pmatrix} M^{(b)} & -R^{-1} \\ (R^{-1})^t & -M^{(a)*} \end{pmatrix}, \quad \zeta \equiv \begin{pmatrix} \bar{z}_b \\ z_a \end{pmatrix}, \quad (40)$$

such that

$$\frac{1}{2} \zeta^t \mathbb{M} \zeta = \frac{1}{2} \left(\bar{z}_b^t M^{(b)} z_b + z_a^t R^{-1t} \bar{z}_b - \bar{z}_b^t R^{-1} z_a - z_a^t M^{(a)*} z_a \right), \quad (41)$$

$$= \frac{1}{2} \sum_{ij} \left(M_{ij}^{(b)} \bar{z}_{b_i} \bar{z}_{b_j} - M_{ij}^{(a)*} z_{a_i} z_{a_j} \right) - \sum_{ij} R_{ij}^{-1} \bar{z}_{b_i} z_{a_j}. \quad (42)$$

Inserting these definitions into Eq. (39), the overlap kernel becomes

$$\langle \phi_a | \phi_b \rangle = (-1)^n \det(R) \int d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b \left(\prod_{i \in \{I^a\}}^{\triangleleft} z_{a_i} \prod_{j \in \{I^b\}}^{\triangleright} \bar{z}_{b_j} e^{\frac{1}{2} \zeta^t \mathbb{M} \zeta} \right). \quad (43)$$

D. Integration over fully-occupied states

We will now integrate variables corresponding to fully occupied states in Eq. (43) by virtue of Eq. (17). In order to do so, we need to move the corresponding differential elements to the very right, which gives a sign factor because of the anticommutation of Grassmann differential elements. For example, such a rearrangement for a single variable in $d_{\triangleleft}^n z_c$ and $d_{\triangleright}^n \bar{z}_c$ gives

$$d_{\triangleleft}^n z_c = dz_{c_1} \cdots \overbrace{dz_{c_k} \cdots dz_{c_n}}^{\downarrow} = \left(\prod_{i \neq k}^{\triangleleft} dz_{c_i} \right) (-1)^{n-k} dz_{c_k}, \quad (44)$$

$$d_{\triangleright}^n \bar{z}_c = d\bar{z}_{c_n} \cdots \overbrace{d\bar{z}_{c_k} \cdots d\bar{z}_{c_1}}^{\downarrow} = \left(\prod_{i \neq k}^{\triangleright} d\bar{z}_{c_i} \right) (-1)^{k-1} d\bar{z}_{c_k}. \quad (45)$$

When there is more than one fully occupied state, the repeated application of this procedure gives

$$d_{\triangleleft}^n z_c = \left(\prod_{i \notin \{I^c\}}^{\triangleleft} dz_{c_i} \right) \left(\prod_{k \in \{I^c\}}^{\triangleright} (-1)^{n-k} dz_{c_k} \right), \quad (46)$$

$$d_{\triangleright}^n \bar{z}_c = \left(\prod_{i \notin \{I^c\}}^{\triangleright} d\bar{z}_{c_i} \right) \left(\prod_{k \in \{I^c\}}^{\triangleleft} (-1)^{k-1} d\bar{z}_{c_k} \right), \quad (47)$$

where in each equation we notice the opposite order for the products over indices corresponding to fully occupied states as compared to other states. Combining Eqns. (46) and (47) gives

$$d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b = \left(\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} \right) \overbrace{\left(\prod_{k \in \{I^a\}}^{\triangleright} (-1)^{n-k} dz_{a_k} \right) \left(\prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j} \right) \left(\prod_{l \in \{I^b\}}^{\triangleleft} (-1)^{l-1} d\bar{z}_{b_l} \right)}^{\downarrow} \quad (48)$$

$$= (-1)^{nr_a} \left(\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} \right) \left(\prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j} \right) \left(\prod_{l \in \{I^b\}}^{\triangleleft} (-1)^{l-1} d\bar{z}_{b_l} \right) \left(\prod_{k \in \{I^a\}}^{\triangleright} (-1)^{n-k} dz_{a_k} \right). \quad (49)$$

The additional sign in Eq. (49) comes from the commutation of variables $k \in \{I^a\}$ to the very right, as indicated in Eq. (48). Defining the sign factor

$$\sigma \equiv (-1)^{\sum_{k \in \{I^a\}} (n+k) + \sum_{k \in \{I^b\}} k}, \quad (50)$$

Eq. (49) finally gives, after a suitable rearrangement of the sign factors

$$d_{\triangleleft}^n z_a d_{\triangleright}^n \bar{z}_b = (-1)^{nr_a + r_b} \sigma \left(\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} \right) \left(\prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j} \right) \left(\prod_{l \in \{I^b\}}^{\triangleleft} d\bar{z}_{b_l} \right) \left(\prod_{k \in \{I^a\}}^{\triangleright} dz_{a_k} \right). \quad (51)$$

The ordering of the differential elements corresponding to indices of fully occupied states are now in the appropriate order with respect to their associated products in Eq. (43) to perform their integration.

By virtue of Eq. (17), the integration over fully occupied levels of the integrand in Eq. (43) gives

$$\int \left(\prod_{k \in \{I^b\}}^{\triangleleft} d\bar{z}_{b_k} \right) \left(\prod_{k \in \{I^a\}}^{\triangleright} dz_{a_k} \right) \left(\prod_{i \in \{I^a\}}^{\triangleleft} z_{a_i} \prod_{j \in \{I^b\}}^{\triangleright} \bar{z}_{b_j} e^{\frac{1}{2} \zeta^t \mathbb{M} \zeta} \right) = \left(e^{\frac{1}{2} \zeta^t \mathbb{M} \zeta} \right)_{\zeta_i=0 \ \forall i \in \{I^b\}, n-i \in \{I^a\}}. \quad (52)$$

With this, Eq. (43) can be rewritten as

$$\langle \phi_a | \phi_b \rangle = (-1)^n (-1)^{nr_a + r_b} \sigma \det(R) \int \left(\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} \right) \left(\prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j} \right) \left(e^{\frac{1}{2} \zeta^t \mathbb{M} \zeta} \right)_{\zeta_i=0 \ \forall i \in \{I^b\}, n-i \in \{I^a\}}, \quad (53)$$

where the integration only runs over variables of indices associated to not fully-occupied states.

E. Integration over the remaining variables

We now define a new matrix \mathbb{M}_r , sub-matrix of \mathbb{M} where rows and columns of indices $i \in \{I^b\}$ of fully occupied states in $|\phi_b\rangle$ and of indices $j+n$, where $j \in \{I^a\}$ are fully occupied levels in $|\phi_a\rangle$, have been removed. The corresponding appropriate vector ζ_r is built from ζ in the same manner, removing components with indices $i \in \{I^b\}$ and $j+n$ such that $j \in \{I^a\}$. The matrix \mathbb{M}_r is skew-symmetric with dimension $N_r \times N_r$, and the vector ζ_r has N_r elements, with $N_r = 2n - (r_a + r_b)$.

For an example where there are two fully occupied states in each quasiparticle vacuum, with indices i, k for the state $|\phi_b\rangle$ and indices j, l for the state $|\phi_a\rangle$, respectively, the matrix \mathbb{M}_r and the vector ζ_r can be schematically represented as

$$\mathbb{M}_r = \begin{array}{c} \begin{array}{cc} \textcolor{red}{i} & \textcolor{red}{k} \\ \textcolor{blue}{j} & \textcolor{blue}{l} \end{array} \\ \left(\begin{array}{cc|cc} \hline & & & \\ \hline & M^{(b)} & & -R^{-1} \\ \hline & & & \\ \hline (R^{-1})^t & & & -(M^{(a)})^* \\ \hline \end{array} \right) \end{array} \quad \zeta_r = \begin{array}{c} \begin{array}{cc} \textcolor{red}{i} & \textcolor{red}{k} \\ \textcolor{blue}{j} & \textcolor{blue}{l} \end{array} \\ \left(\begin{array}{cc} \hline \bar{z}_b \\ \hline z_a \\ \hline \end{array} \right) \end{array} \quad (54)$$

$$(55)$$

$$(56)$$

where labeled rows and columns have been removed from the original objects \mathbb{M} and ζ . Using the submatrix \mathbb{M}_r and subvector ζ_r , Eq. (53) can be rewritten as

$$\langle \phi_a | \phi_b \rangle = (-1)^n (-1)^{nr_a + r_b} \sigma \det(R) \int \left(\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} \right) \left(\prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j} \right) \left(e^{\frac{1}{2} \zeta_r^t \mathbb{M}_r \zeta_r} \right). \quad (57)$$

In order to apply the Pfaffian formula Eq. (A4), the order of $\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i}$ has to be reversed, such that the differential elements in Eq. (57) are in the appropriate order with respect to the matrix \mathbb{M}_r . This is achieved by reversing the order of $\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i}$

$$\prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} = (-1)^{(n-r_a)(n-r_a-1)/2} \prod_{i \notin \{I^a\}}^{\triangleright} dz_{a_i}. \quad (58)$$

The sign factor from the reversal of the product $z_1 \cdots z_n = (-1)^{n(n-1)/2} z_n \cdots z_1$ can be obtained by induction. The differential elements are now in the appropriate order

$$d_{\triangleright}^{N_r} \zeta_r = \prod_{i \notin \{I^a\}}^{\triangleright} dz_{a_i} \prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j} \quad (59)$$

$$= (-1)^{(n-r_a)(n-r_a-1)/2} \prod_{i \notin \{I^a\}}^{\triangleleft} dz_{a_i} \prod_{j \notin \{I^b\}}^{\triangleright} d\bar{z}_{b_j}, \quad (60)$$

such that we can now integrate the remaining variables using the Pfaffian formula, Eq. (A4),

$$\langle \phi_a | \phi_b \rangle = (-1)^n (-1)^{nr_a + r_b} \sigma \det(R) (-1)^{(n-r_a)(n-r_a-1)/2} \int d_{\triangleright}^{N_r} \zeta_r e^{\frac{1}{2} \zeta_r^t \mathbb{M}_r \zeta_r} \quad (61)$$

$$= (-1)^{n(n+1)/2} (-1)^{r_a(r_a-1)/2} (-1)^{r_a + r_b} \sigma \det(R) \text{pf}(\mathbb{M}_r). \quad (62)$$

This formula, however, assumes N_r to be even, see appendix A. When N_r is odd, $|\phi_a\rangle$ and $|\phi_b\rangle$ have in fact different *number parity* [20]. In that case, the overlap $\langle \phi_a | \phi_b \rangle$ is automatically zero. From the definition of the Pfaffian, which by definition is zero for skew-symmetric matrices of odd rank, we can thus notice that formula Eq. (57) can still be applied. In particular, $(-1)^{r_a + r_b}$ will always be one except when multiplied by zero, allowing to drop this sign factor in the final formula. We thus summarize the final expression for the overlap as

$$\langle \phi_a | \phi_b \rangle = s_n s_{r_a} \sigma \det(R) \text{pf}(\mathbb{M}_r), \quad (63)$$

where

$$s_n = (-1)^{n(n+1)/2}, \quad (64)$$

$$s_{r_a} = (-1)^{r_a(r_a-1)/2}, \quad (65)$$

$$\sigma = (-1)^{\sum_{k=1 \dots r_a} (n + i_{k_a}) + \sum_{k=1 \dots r_b} i_{k_b}}. \quad (66)$$

The sign factors depend on the number of states in the single-particle bases n , the number of fully occupied states r_a in a , and the indices i_{k_c} of fully occupied states in the bases $c = a, b$.

Equation (63) provides the generalization of Eq. (7) of Ref. [7] to the overlap between different quasiparticle

vacua with an arbitrary number of fully occupied single-particle states. In particular, it can be applied to overlaps that involve an odd number of blocked quasiparticle states, a case not considered at all in Refs. [7, 9], and for the special case of symmetry restoration only in Ref. [10]. Moreover, when an even number of particles is fully occupied (either for blocked $2n$ quasiparticle states, or as a result of the minimization, or both), Eq. (63) provides a formally justified alternative to the regularization of the matrix \mathbb{M} performed in [9].

Besides this important generalization, there is another noteworthy difference to previous work by Robledo [7, 9]. Indeed, Eq. (63) is directly expressed in the single-particle bases of $|\phi_a\rangle$ and $|\phi_b\rangle$, respectively, that allow for the most compact representation of these quasiparticle vacua. In particular, Eq. (63) can also be applied without invoking a complete single-particle basis spanning the single particle subspace $a \cup b$, cf. the discussions above. However, as explained there, if the matrix R is singular, one is forced to complete each single-particle basis until $\det(R) \neq 0$ is achieved.

For quasiparticle vacua for which there are no fully occupied states in their respective single-particle basis, it is easy to show that Eq. (7) of Ref. [7] is recovered.

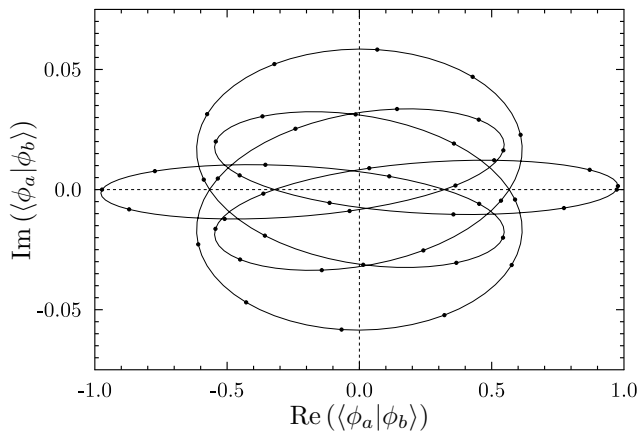


FIG. 1: Real and imaginary parts of the overlap without particle-number projection for the lowest one-quasiparticle state in ^{25}Mg obtained with SHH. The Euler angles α and β are held fixed at values of $\alpha = 1.25^\circ$ and $\beta = 7.17^\circ$, whereas γ is varied in the interval $[0, 720^\circ]$ with a discretization of 288 points. Filled circles on the curve represent a discretization of 48 points in the interval $[0, 720^\circ]$, which is sufficient to converge observables. Note the difference in scale of real and imaginary parts.

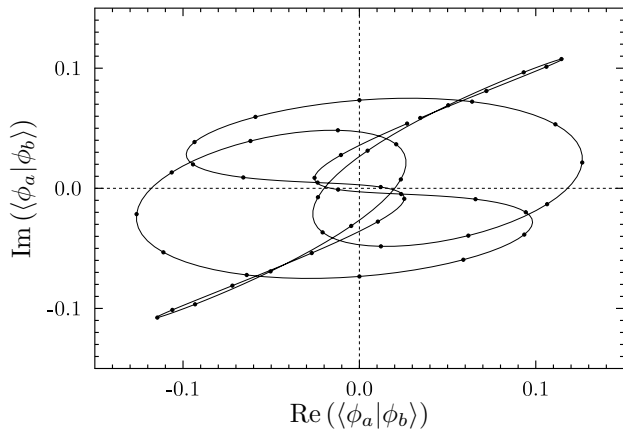


FIG. 2: Same as Fig. 1, but for $\alpha = 43.75^\circ$ and $\beta = 71.94^\circ$.

V. SOME ILLUSTRATIVE EXAMPLES

The determination of the phase of the overlap by the widely used techniques that rely on a Taylor expansion of the overlap around a matrix element of known phase [5, 6, 14] works very well when restricting the calculations to time-reversal invariant HFB states. However, it becomes increasingly difficult when time-reversal is broken, as it happens for odd- A or odd-odd nuclei, or for states obtained with cranked HFB, cf. the examples discussed in Refs. [5, 6, 21].

We have implemented Eq. (63) into our numerical codes for particle-number and angular-momentum restored GCM calculations based on triaxial HFB states [15, 16], using the routines for the calculation of the Pfaf-

fian of Ref. [22]. We now present three examples where techniques to follow the overlap through Taylor expansion might fail and the direct calculation of the overlap becomes a necessity. These illustrations will show trajectories in the complex plane of overlaps of quasi-particle vacua as obtained during angular-momentum projection

$$\langle \phi_a | \phi_b \rangle = \langle \varphi | \hat{R}(\alpha, \beta, \gamma) | \varphi \rangle, \quad (67)$$

where \hat{R} is the rotation operator that depends on the three Euler angles α , β , and γ .

The first two examples are presented in Figs. 1 and 2. They illustrate the trajectory of the overlap in the complex plane when varying the Euler angles γ when projecting the lowest self-consistent one-quasiparticle state of ^{25}Mg , for two different combinations of α and β . The first one, Fig. 1, illustrates that real and imaginary parts of the overlap can vary on quite different scales. In this particular case, most of the modulus of the overlap is carried by the real part, and the phase of the overlap is most of the time either close to zero or close to $\pm\pi$. Unless the discretization of the Euler angles is carefully adapted, the phase of the overlap might change by almost π when crossing the imaginary axis, which is very difficult to distinguish from a discontinuity by π encountered when having lost the phase. The second example, Fig. 2, obtained for a different combination of Euler angles α and β , shows that the trajectory of the overlap in the complex plane may exhibit cusps, which might again be difficult to resolve when discretizing Euler angles.

In Fig. 3, we present the trajectory of the overlap of a high-spin state in ^{24}Mg , obtained from cranked HFB+Lipkin Nogami [23]. The two inserts illustrate that variations may occur on very different scales with quite involved structures.

These three examples demonstrate that a Taylor-expansion-based algorithm to determine unambiguously the sign of the overlap may become difficult in applications that use time-reversal invariance breaking quasi-particle vacua. Indeed, it should be able to resolve discontinuities or cusps, or other involved structures. The latter might happen at very different scales, and the discretization must be chosen in order to account for all these details. Furthermore, we expect the complexity of such trajectories to increase with increasing intrinsic angular momentum. A direct determination of the overlap is thus a considerable improvement not only from a formal point of view, but also from the perspective of the complexity of reliable algorithms for the computation of the overlap on the one hand and of computing time on the other hand, as it will often allow for the use of a smaller number of combinations of Euler angles in angular-momentum projection.

VI. DISCUSSION AND OUTLOOK

To summarize our main findings

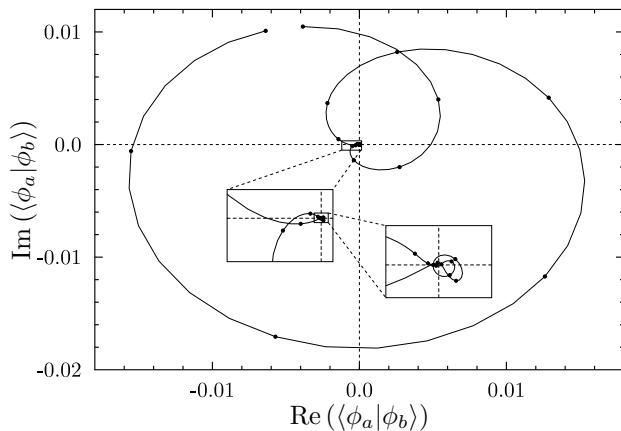


FIG. 3: Real and imaginary parts of the overlap without particle-number projection for the cranked $I = 8\hbar$ state in ^{24}Mg obtained with SHH. The Euler angles α and β are held fixed at values of $\alpha = 23.75^\circ$ and $\beta = 66.96^\circ$, respectively, whereas γ is varied in the interval $[0, 360^\circ]$ with a discretization of 144 points. The inserts amplify the zone at very small overlaps, whereas filled circles on the curves represent a discretization of 24 points in the interval $[0, 360^\circ]$, which is sufficient to converge observables.

1. An extension of the Thouless parameterization of quasiparticle vacua with completely filled single-particle states allows to calculate the overlap directly in a formalism based on Grassmann algebra and coherent states similar to the one outlined in Ref. [7], but in such a manner that fully occupied or empty single-particle levels are automatically taken care of without any need for the manipulation (or regularization) of matrices elaborated in Ref. [9].
2. This extension of the Thouless expression allows to handle all possible quasiparticle vacua that have completely filled states, i.e. also 1-, 2-, ... n -quasiparticle states, not just quasiparticle vacua that can be expressed as limits of fully-paired quasiparticle vacua as in Ref. [9].
3. The handling of blocked states is not restricted to pure symmetry restoration as the one proposed in Ref. [10], and therefore can be also applied when the non-rotated left and right states are different, which is necessary for GCM calculations.
4. Our final expression for the overlap allows for the calculation of the overlap of two quasiparticle vacua that are expressed in two different single-particle bases that do not span the same sub-space of the Hilbert space of single-particle states. The knowledge of a complete basis spanning both single-particle bases is not needed, as compared to Ref. [9]. In this way, the technique can be directly implemented in codes that use a coordinate space representation of the quasiparticle vacua in terms of their canonical single-particle bases [13–16].

The expression has been implemented into our numerical codes for particle-number and angular-momentum restored GCM calculations based on triaxial HFB states using the full space of occupied single-particle states [15, 16]. It has been extensively tested for symmetry restoration and for the calculation of non-diagonal matrix elements for symmetry-restored GCM calculations without encountering cases where it fails.

By contrast, the technique “to follow the phase” from Ref. [5, 14], or the one to follow the overlap in the complex plane from Ref. [6] require often to use a very fine discretization to resolve the sign ambiguity when projecting on angular momentum as soon as time-reversal invariance of the HFB states is broken. In particular, it may become necessary to use a discretization of the integrals over Euler or gauge angles that are much finer than what is actually needed to converge observables. In addition, the direct calculation of the overlap also has the advantage to avoid complicated coding for the set-up of a reliable Taylor-expansion-based algorithm, in particular since reliable routines to compute pfaffians are available [22]. Finally, in the general case of configuration mixing where there might not be a symmetry that establishes a reference sign for the overlap, such a direct calculation of the overlap could become to be mandatory.

In summary, we report an expression for the overlap between arbitrary quasiparticle vacua that is easy to calculate and that is very robust in realistic applications. It is a key ingredient for the extension of symmetry restoration and Generator Coordinate Method-type calculations to angular-momentum-optimized states, either by cranking, or by blocking.

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Appendix A: Some remarkable Gaussian integrals over Grassmann variables

For the readers’ convenience, we give the identities that represent determinants and pfaffians as integrals over Grassmann variables using our convention for the order of the differential elements, Eq. (22).

1. Determinant

The first one is the determinant identity that is defined, for a given matrix M , as

$$\det(M) = \int \prod_i (dz_i d\bar{z}_i) \exp \left(\sum_{i,j=1}^n \bar{z}_i M_{ij} z_j \right) \quad (\text{A1})$$

$$= (-1)^n \int d_{\mathbb{P}}^n \bar{\mathbf{z}} d_{\mathbb{Q}}^n \mathbf{z} \exp \left(\sum_{i,j=1}^n \bar{z}_i M_{ij} z_j \right) \quad (\text{A2})$$

where the first equation is the expression from Ref. [19], p. 13, Eq. (1.67), and the second uses an alternative convention in the ordering of differential elements. The latter differs by a sign because of the anticommutation of \mathcal{G} -variables.

2. Pfaffian

The second one is the Pfaffian identity that is defined for a skew-symmetric matrix A of dimension $2n \times 2n$, as

(see [19], p.15, Eq. (1.80)):

$$\text{pf}(A) = \int dz_{2n} \cdots dz_2 dz_1 \exp \left(\frac{1}{2} \sum_{i,j=1}^{2n} z_i A_{ij} z_j \right) \quad (\text{A3})$$

$$= \int d_{\mathbb{P}}^{2n} \mathbf{z} \exp \left(\frac{1}{2} \sum_{i,j=1}^{2n} z_i A_{ij} z_j \right). \quad (\text{A4})$$

To obtain the correct sign, it is crucial that the differential elements are in the same order as the indices of the matrix A_{ij} . This implies sometimes to make some manipulations to bring the entire expression into the proper form, as for example between Eq. (57) and Eq. (61).

As can be easily seen, this definition is only valid for matrices A of *even* rank. The determinant and the Pfaffian of a skew-symmetric matrix A are related by

$$[\text{pf}(A)]^2 = \det(A). \quad (\text{A5})$$

As the determinant of a skew-symmetric matrix of *odd* rank is always zero, the pfaffian of such a matrix is defined to be zero as well.

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